ABSTRACT

The invention relates to novel proteins with novel integrin and I domain activity and nucleic acids encoding these proteins. The invention further relates to the use of the novel proteins in the treatment of integrin related disorders.

Table 1

Table 1. Computationally designed mutants[a]

	WT	ido1q	ido1r	ido2r	jlm2r
Backbone			Energy[b]		
1ido	-1037	-1145	-1138	-1116	-678
1jlm	-1059	+82758	-840	-1000	-1086
Position			Residues		
139	I	-	-	V	-
153	M	-	-	A	-
156	F	L	W	-	-
157	V	-	-	I	-
160	V	I	-	-	-
199	V	I	I	I	-
215	I	L	L	-	V
219	V	-	-	-	I
223	F	-	-	-	L
238	V	F	F	I	I
239	V	L	L	L	-
240	I	L	L	-	-
259	A	L	L	-	-
269	I	L	-	-	-
271	V	F	-	-	-
287	I	V	V	V	-
299	V	A	I	I	-
308	I	V	-	-	-

[a] Mutants are named according to the structure that was stabilized (ido or jlm), the solvation potential used (1 or 2) and the definition of core residues (q or r).

[b] The lowest energy rotamer configuration was calculated for each sequence in the 1ido structure, and cross-calculated in the 1jlm structure, using both solvent potentials; all 50 core residues were used in order to make the q and r energies comparable. Results are shown for solvent potential 1 and were similar for potential 2. A severe clash of the side-chain of F271

with the backbone caused the high energy of the 1q sequence in the 1jlm structure; no movement of the backbone is allowed by the design method.

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